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Structure Investigation of MAIPO₄-5

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Beamline: X7B

Introduction: The microporous aluminophosphate AIPO₄-5 is made in hydrothermal synthesis at temperatures up to 200°C from amorphous aluminophosphates containing organic amines as template molecules. The structure is of the AFI type (1), and several structural investigations have been reported. The structure of AIPO₄-5, AFI, with the template tetrapropylammonium hydroxide (2) and the template triethylamine (3) has been reported using single crystal and neutron powder diffraction data, respectively. Recently, the absolute configuration and domain structure of AIPO₄-5 was studied by single crystal synchrotron X-ray diffraction analysis (4). When the compound is heated at temperatures up to 700°C, the template is removed, and the structure of the calcined product has been described using neutron powder diffraction data (3, 5). Al in AIPO₄-5 can be substituted by the divalent metal ions Mg²⁺, Mn²⁺, Co²⁺, and Zn²⁺, and the substitution is assumed to take place in the framework. The degree of substitution is in general low.

Results: The present investigation was made to study the degree of Co-substitution of Al in CoAIPO₄-5. The compound was made in a hydrothermal synthesis at 188°C from a reaction mixture where molar ratios of the elements were: Co: 0.20, Al: 1.80, P: 2.00, template triethylamine: 1.60, F: 0.8. Hydrofluoric acid was used as a mineralizer. The crystal used in the measurements had the dimensions: 0.025 x 0.025 x 0.075 mm. Single crystal measurements were made on the MAR-diffractometer at beam line X7B. A data set was measured using the wavelength $\lambda = 0.9269 \text{ \AA}$, and a set was measured at $\lambda = 1.3568 \text{ \AA}$, which is close to the absorption edge of Co. The two sets of data were used simultaneously with the least squares program SHELXL97 (6) to determine the degree of Co substitution on the Al-sites in the framework. However, the value could not be determined from this data. An additional data set will be obtained nearer to the absorption edge of Co to resolve this problem. In a similar investigation of the Zn substitution in ZnAIPO₄-5 (7) the Zn substitution on the Al-sites was found to be 1.5%.

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